Assessing Diffusion Transport Modeling in Premixed Flames

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Abstract

Turbulent combustion drives most practical combustion devices such as internal combustion and gas turbine engines. The fundamental combustion physics in these devices is complex because of the parallel diffusion of mass, heat, and momentum. However, turbulent combustion occurs at high temperatures and pressures and experimental measurement tools are often unable to withstand these conditions and are insufficient to fully characterize these physics. Further complicating the study of these flames, modeling the multicomponent mass diffusion present in these flames has been computational cost prohibitive due to the challenges involved in computing diffusion coefficients. As a result, mixture-averaged diffusion treatments or simpler methods are used to avoid these costs. However, the accuracy and appropriateness of the mixture-averaged diffusion model has not been verified for three-dimensional turbulent premixed flames. This dissertation presents a fast, low-memory algorithm for implementing full multicomponent mass diffusion in direct numerical simulation of turbulent flames. In addition, it presents the first assessment of the accuracy and appropriateness of the mixture-averaged diffusion approximation in these flames. Mixture-averaged diffusion approximation is observed to overpredict the magnitude of mass diffusion fluxes by as much as 50% in regions of high flame curvature. These errors seem to result in a fundamental change to the average internal flame structure and alter global flame statistics such as the turbulent flame speed. Considering the computational efficiency of the proposed method, these conclusions raise questions on the continued use of the mixture-averaged and other diffusion assumptions for the DNS of reacting flows.

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